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Exploring the utility of a multivariate soil hyperspectral reflectance model for estimating soil moisture using sentinel-2 Data

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Abstract

Accurate and spatially transferable estimation of soil moisture is critical for sustainable agriculture, water resource management, and drought monitoring, particularly in data-scarce semiarid regions. However, soil moisture retrieval from optical satellite data remains challenging due to heterogeneous soil conditions and limited model generalizability, especially when interactions between soil moisture and clay content are neglected. This study presents a physically informed, simulation-based multivariate framework for estimating soil moisture from freely available Sentinel-2 multispectral imagery that explicitly accounts for soil clay content and its interaction with moisture. A Monte Carlo look-up table comprising 100,000 synthetic soil reflectance spectra was generated under varying soil moisture and clay conditions and resampled to Sentinel-2 spectral bands. Soil moisture-sensitive spectral band combinations, ratios, and newly developed soil moisture indices were derived and used to train machine learning models, which were evaluated using group-aware cross-validation to assess spatial robustness and transferability. Model application across multiple agricultural sites in South Africa's Eastern Cape and Limpopo provinces, regions geographically distinct from calibration areas and spanning contrasting ecological and climatic conditions demonstrated high predictive performance (R^2 up to 0.91; RMSE as low as 0.71) and strong spatial transferability. The results indicate that explicitly integrating soil property interactions within a synthetic spectral modeling framework substantially improves Sentinel-2–based soil moisture estimation. The proposed approach advances operational optical remote sensing of soil moisture by bridging physically consistent spectral simulations and scalable multispectral observations, providing a transferable methodology for precision irrigation, drought early warning, and sustainable agricultural water management in semiarid environments.